

ENHANCING STRUCTURE DIAGRAM GENERATION

ABSTRACT OF THE DISCLOSURE

A method and a system are provided for enhancing structure diagram generation ("SDG"). In SDG, aesthetic two-dimensional ("2-D") coordinates for use in a diagrammatic representation ("diagram") of a molecule are derived from a connection table for the molecule. SDG may also improve the aesthetic qualities of a chemical structure diagram having existing coordinates, if available. SDG is enhanced by expressing the symmetry present in the molecule, by making use of symmetry in the 2-D dynamics used to lay out rings and chains, by construction of bridges using an open polygon method together with a potential function, and by an elegant approach to the relative positioning of molecules ("free rectangle method").